THE SHIFT:
Properties and recommendations for practical use

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Abstract. In mechanics of structures as well as in other domains of engineering, the probabilistic models often have to be computed by simulation. One of the reasons is that the stochastic calculus involved in non linear representations yields rarely explicit formulas. Usually these simulations use, for each sample, a large number of calls to the random function, in this case the simulation by the shift, whose field of application is as wide as that of Monte Carlo method, is particularly relevant.

The theoretical features, the implementation and the specific advantages of this method have been taught in a course of the author at Paris VI University in 1988 and are detailed in the book with D. Lépingle [BL].

I. Other known methods of simulation

Let us begin by the presentation of the methods to be compared with the shift.

A. The Monte Carlo method

For computing the expectation $\mathbb{E}(X)$ of a random variable X, it consists of
a) representing X as a random variable defined on the probability space

$$([0,1]^s, \mathcal{B}[0,1]^s, dx_1 dx_2 \cdots dx_s)$$

with s finite or infinite,
b) imitating independent random samples of points of $[0,1]^s$,

$$(U_{11}, U_{12}, \ldots, U_{1s}) \ , \ (U_{21}, U_{22}, \ldots, U_{2s}) \ , \ldots , \ (U_{n1}, U_{n2}, \ldots, U_{ns}) \ , \ldots$$

c) and applying the law of large numbers

$$\mathbb{E}(X) = \lim_{N \uparrow \infty} \frac{1}{N} \sum_{n=1}^{N} X(U_{n1}, U_{n2}, \ldots, U_{ns}).$$

Comments

• The step a) is the art of using the *algorithms of simulation*. It is theoretically possible to take $s = 1$, but practically, the dimension s, finite or infinite, is rather naturally given and is difficult to reduce. The main reference for these algorithms is [Devroye 86]. It is worth to note that this operation of representing a random variable X on the cube $[0,1]^s$ (s finite or not) can be effectively performed in very much more cases than those where the law of X is known by an explicit formula. This is, in particular, due to the *rejection method* which allows an exact simulation of a random variable even when its density is only known by a sequence of approximations.

• The step b) is the generation of pseudo random numbers. The imitation of randomness cannot be perfect. It has been theoretically proved by logicists, especially by Martin Löf. Practically extremely good generators are available with gigantic period. They are obtained by testing the production algorithms through statistical tests and eliminating those who behave badly. The tests are quite numerous (see [Niederreiter 1978], Knuth 1981, Marsaglia 1985, Ripley 1987, Fushimi 1988, Altman 1988, Anderson 1990, and other references given in [BL])
• The class of functions to which the Monte Carlo method applies is theoretically all functions in $\mathcal{L}^1([0,1]^s, dx)$ (here dx is the product probability measure). Practically, it is safe to restrict the method to bounded functions. Nevertheless the irregularity of the function is not limited.
• The speed of convergence is given for X in L^2, hence for X bounded, by the law of iterated logarithm

$$\limsup_N \frac{1}{\sigma\sqrt{2N\log\log N}}\left(\sum_{n=1}^N X(U_{n1}, U_{n2}, \ldots, U_{ns}) - \mathbb{E}X\right) = 1$$

where σ^2 is the variance of X.

There are also global estimates of the type Cramer-Chernov (X bounded)

$$\mathbb{P}(\frac{1}{N}\sum_{n=1}^N X(U_{n1}, U_{n2}, \ldots, U_{ns}) \geq \mathbb{E}X + \varepsilon) \leq e^{n\psi(\varepsilon)}$$

which are in connexion with large deviation theory.

B. Quasi-Monte Carlo methods

The step a) is preserved, but b) and c) are replaced by
b') choosing an equidistributed sequence (ξ_n) on $[0,1]^s$,
c') putting

$$\mathbb{E}(X) = \lim_{N\uparrow\infty} \frac{1}{N}\sum_{n=1}^N X(\xi_n).$$

Comments • This method requires the random variable to be represented on $[0,1]^s$ by a *Riemann integrable function* i.e. a bounded function whose discontinuity points belong to a negligible set, or equivalently such that $\forall\varepsilon > 0$ continuous functions u, v exist such that $u \leq X \leq v$, $\int(v-u)dx \leq \varepsilon$.

Often the function obtained on $[0,1]^s$ by the step a) is Riemann integrable already, so this fact brings no restriction.

The non-Riemann integrable functions encountered in practice, come from stochastic calculus related to Brownian motion for which quasi-Monte Carlo methods are not yet relevant.
• The speed of these methods using low discrepancy sequences [cf Niederreiter 1978] is impressive in low dimension. A great advantage is also that the rate of convergence is given by a deterministic criterion — the Koksma-Hlawka formula — allowing to produce the numerical value of the computed expectation with an explicit accuracy (cf [BL] Chapter 2C). But this speed is decreasing when the dimension increases, so that for large dimensional simulations these methods are at present irrelevant (see [BL] for the study of the realm of efficiency of these methods).

II. The shift method

A. The infinite dimension in practice

Because the shift method is particularly relevant in large or infinite dimension, it is important to emphasize the fact that *the case of infinite dimension is practically the most frequent.*

Indeed, most often, in the simulation, the number of calls to the random function, although finite, is itself random and unbounded. A typical example is the computation of the expectation of a stopping time of a Markov chain, e.g. the entrance time in a given set.

But even for a finite dimensional probabilistic model the step a) will lead to the infinite dimension if the rejection method is used, and practionners know how rejection is often unavoidable.

B. The principle of the shift method

It is based on the pointwise ergodic theorem instead of the law of large numbers.

Let X be a random variable simulated under the form

$$X = F(U_1, U_2, \ldots, U_n, \ldots)$$

where yhe U_i's are i.i.d. random variables uniformly distributed on $[0,1]$. In other words the U_i's are the coordinate mappings from $[0,1]^\infty$ equipped with the product Lebesgue measure to each factor. The method consists of putting

$$\mathbb{E}(X) = \lim_{N\uparrow\infty} \frac{1}{N}[F(U_1, U_2, \ldots) + F(U_2, U_3, \ldots) + \cdots + F(U_N, U_{N+1}, \ldots)]$$

instead of using in the case of the Monte Carlo method a double sequence of calls:

$$\mathbb{E}(X) = \lim_{N\uparrow\infty} \frac{1}{N}[F(U_{11}, U_{12}, \ldots) + F(U_{21}, U_{22}, \ldots) + \cdots + F(U_{N1}, U_{N2}, \ldots)]$$

The theorem of Birkhoff says that the shift method converges almost surely and in L^1 as soon as X is in L^1 and in L^p as soon as X is in L^p $1 \leq p < \infty$.

C. General implementation manner

Suppose we have written a procedure able to give us a sample of the probabilistic model we are studying.

Instead of writing the main program using this procedure successively N times and doing the average, we shall write the main program using N times the procedure after initialisation and shifting one step the random function each time.

The economy on the pseudo-random numbers generator is evident.

D. Fine implementation for efficiency

In order to exploit the full strength of the method the maximum amount of information of the preceding sample has to be kept for the following one.

This can be done very efficiently by *pointers*. Let us take the example of a Markov chain for the explanation.

Let us consider a Markov chain X_n with values in $\mathbb{R}^d$ which is simulated on $[0,1]^\infty$ in the following way:

$$X_{n+1} = F(X_n, n, U_{n+1}), \quad X_0 = x$$

where F is a map from $\mathbb{R}^d \times \mathbb{N} \times [0,1]$ into $\mathbb{R}^d$, and where the U_n's are, as before, the coordinate mappings of the cube $[0,1]^\infty$ to its factors.

Let us suppose we want to compute the expectation of a functional of the process X, for instance $\mathbb{E}[G(X_T, T)]$ where G is a given bounded function and T the hitting time in the set $A \subset \mathbb{R}^d$: $T = \inf\{n > 0;\ X_n \in A\}$.

Denoting θ the shift operator on $[0,1]^\infty$ defined by

$$U_n \circ \theta = U_{n+1},$$

the ergodic theorem writes

$$\mathbb{E}[G(X_T, T)] = \lim_{N \uparrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} G(X_T, T) \circ \theta^n.$$

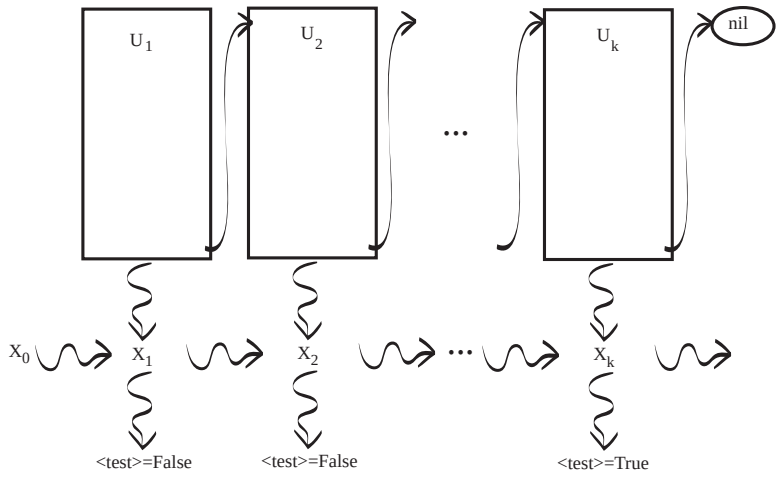
The use of pointers can be explained as follows. In order to apply the preceding formula we have to compute$G(X_T, T)$ on successive points $\omega, \theta(\omega), \theta^2(\omega), \ldots,$ in $[0,1]^\infty$. These points are sequences of points in $[0,1]$:

$$\begin{array}{rcl} \omega & = & (U_1(\omega), U_2(\omega), \ldots, U_k(\omega), \ldots) \\ \theta(\omega) & = & (U_2(\omega), U_3(\omega), \ldots, U_{k+1}(\omega), \ldots) \end{array}$$

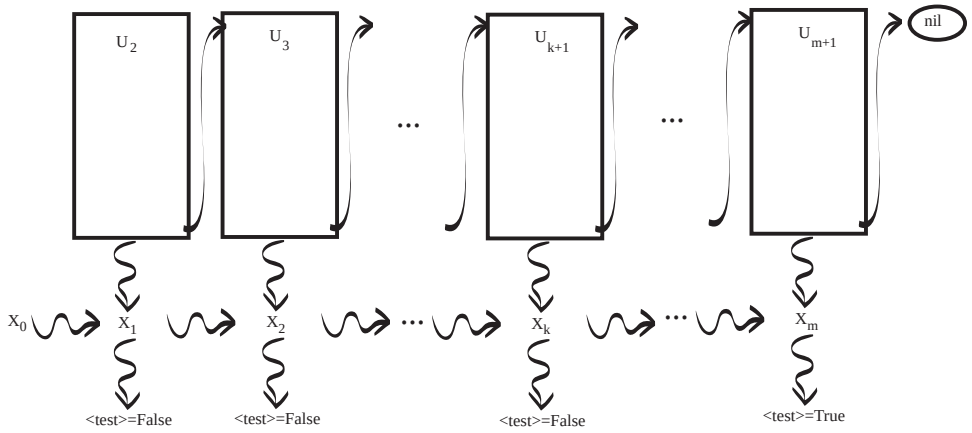
If, as we suppose, the stopping time T is finite, we need only to compute a finite length of each of these sequences: the sequence ω is computed until $T(\omega)$ which is given by the test

$$< \text{test} > \left\{ \begin{array}{rcl} X_k(\omega) \text{ still outside } A & \Rightarrow & k < T(\omega) \\ X_k(\omega) \in A \text{ for the first time} & \Rightarrow & k = T(\omega) \end{array} \right.$$

Suppose we have picked out the sequence $\omega = (U_1, U_2, \ldots)$ and we have put the numbers $U_1, U_2, \ldots$ in pointers as in the following figure:



The sequence $\theta(\omega) = (U_2, U_3, \ldots)$ is already partially chosen: either it is long enough or it must be lengthened, in which case we have the new scheme:



In these figures the arrows represent computations to do, essentially to compute

$$X_{n+1} = F(X_n, n, U_{n+1})$$

When we compute $F(x, n, y)$ however, only the variable x is new (and n becomes $n+1$) and *partial computations depending only on y can be stored in the box of U_n*. This storage must of course be made while we are lengthening the sequence as explained above.

Clearly this storage of partial computations cannot be done in the Monte Carlo method.

E. Theoretical results on the rate of convergence

We dont go into the details of these results here, see [BL] for mathematical proofs.

There is no standard rate of convergence valid for every function in L^2. Nevertheless in practice usual functions belong to a class called the Gordin class in which a law of iterated logarithm holds.

This law of iterated logarithm involves a coefficient different from the variance, which can be either bigger or smaller than the variance even in the finite dimensional case. So even for integration in finite dimension the shift can be faster than Monte Carlo.

From a practical point of view the possibility of storage of partial computations is the dominant phenomenon.

F. Numerical example

The simulated device is a transport particles problem. A particle arrives in 0 coming from the real negative axis and enters into the square $[0,1] \times [-\frac{1}{2}, \frac{1}{2}]$ where it goes in straight lines during a random distance which follows an exponential law with parameter λ, then it splits into two similar directions uniformly distributed on $[-\frac{\pi}{2}, \frac{\pi}{2}]$ with respect to the direction of the preceding particle, and they behave as the initial particle provided they are inside the square. The quantities to be computed are the mean number of splittings and the mean number of particles leaving the cube by the righthand side.

The following results have been obtained by simulating 500 000 samples by the Monte Carlo method (MC) and the shift method (Sh)

parameter	0.980		0.960		0.940		0.920		0.900	
method	MC	Sh	MC	Sh	MC	Sh	MC	Sh	MC	Sh
mean number of splittings	2.78	2.79	2.92	2.93	3.12	3.11	3.34	3.31	3.60	3.58
mean number of particles through the righthand side	3.97	4.00	4.36	4.38	4.95	4.90	5.68	5.62	6.72	6.65
mean number of calls to the random function	24.5	4.9	27.4	4.9	32	4.9	37	5	46	5
ratio of the duration of the programs MC/Sh	2.04		2.19		2.31		2.40		2.46	

III. Recommendations

To become an expert in the art of using the shift, it is essential to keep in mind that *the rate of convergence depends on the order of the calls*

Let us take a finite dimensional example: Let f be a bounded function from $[0,1]^d$ into $\mathbb{R}$. The integral of f can be obtained by the shift by putting

$$\mathbb{E}f = \lim_{N\uparrow\infty} \frac{1}{N}[f(U_1,\ldots,U_d) + f(U_2,\ldots,U_{d+1}) + \ldots + (U_N,\ldots,U_{N+d})]$$

Now we can also permute the coordinates defining with the permutation σ

$$f_\sigma(x_1,\ldots,x_d) = f(x_{\sigma(1)},\ldots,x_{\sigma(d)})$$

and apply the shift to f_σ.

The rate of convergence *will be different* in general, so that there are $d!$ different manners of applying the shift.

In finite dimension these different manners give roughly speaking the same order of rate (see [BL] for a detailed study)

But in infinite dimension it is quite different and for simulating the expectation of a functional of a random process this becomes very important: *The idea of discretization of the process and shifting along the time is one of the* **worse** *way.* Good implementations for functionals of Brownian motion and for solution to stochastic differential equations are given in [BL Chapter V].

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